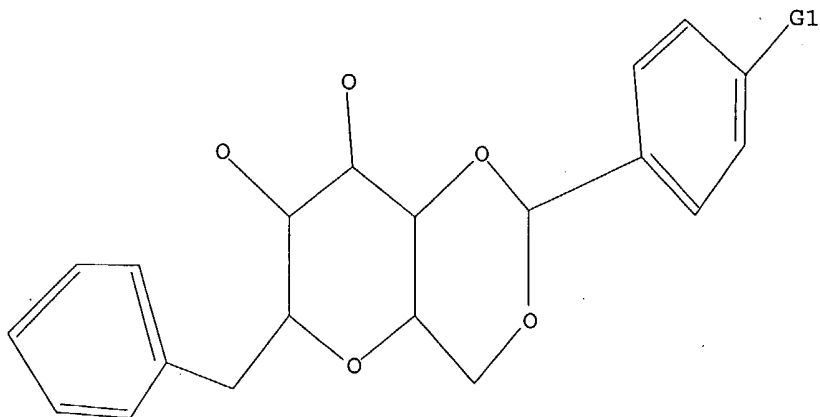


11/01/2004

STR



G1 Cl,Br,F

2 SEA SSS FUL L1

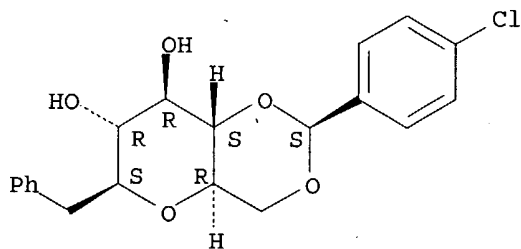
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L2 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 727416-83-3 REGISTRY  
 ED Entered STN: 16 Aug 2004  
 CN D-glycero-D-gulo-Heptitol, 2,6-anhydro-5,7-O-[(S)-(4-chlorophenyl)methylene]-1-deoxy-1-phenyl- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C20 H21 Cl O5  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: PREP (Preparation)

## Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2
C402-C50	OCOC3-OC5	6-6	C703	591.449.1	1

Absolute stereochemistry. Rotation (+).



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	973	pH 1	(1) ACD
Bioconc. Factor (BCF)	973	pH 4	(1) ACD
Bioconc. Factor (BCF)	973	pH 7	(1) ACD
Bioconc. Factor (BCF)	973	pH 8	(1) ACD
Bioconc. Factor (BCF)	972	pH 10	(1) ACD
Boiling Point (BP)	565.4+/-50.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVP)	89.34+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	295.7+/-54.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	5		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	4789	pH 1	(1) ACD
Koc (KOC)	4789	pH 4	(1) ACD
Koc (KOC)	4789	pH 7	(1) ACD
Koc (KOC)	4789	pH 8	(1) ACD
Koc (KOC)	4784	pH 10	(1) ACD
logD (LOGD)	4.23	pH 1	(1) ACD
logD (LOGD)	4.23	pH 4	(1) ACD
logD (LOGD)	4.23	pH 7	(1) ACD
logD (LOGD)	4.23	pH 8	(1) ACD
logD (LOGD)	4.23	pH 10	(1) ACD
logP (LOGP)	4.235+/-0.521		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	376.83		(1) ACD
pKa (PKA)	12.98+/-0.20	Most Acidic	(1) ACD
Vapor Pressure (VP)	1.28E-13 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

ACCESSION NUMBER: 141:134051 CA  
 TITLE: Bicyclic carbohydrates as antiprotozoal bioactive for the treatment of infections caused by parasites  
 INVENTOR(S): Sas, Benedikt; Van Hemel, Johan; Vandenkerckhove, Jan; Van Hemel, Johan; Peys, Eric; Van Der Eycken, Johan; Ruttens, Bart; Van Hoof, Steven  
 PATENT ASSIGNEE(S): Kemin Pharma Europe B.V.B.A., USA  
 SOURCE: PCT Int. Appl., 26 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 INT. PATENT CLASSIF.:  
 MAIN: A61K  
 CLASSIFICATION: 1-5 (Pharmacology)  
 Section cross-reference(s): 33  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004062590      A2      20040729      WO 2004-US311      20040107

W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AU, AZ, AZ, BA, BB,  
BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR,  
CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG,  
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ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ,  
KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN,  
MW, MX, MX, MZ

US 2004180838      A1      20040916      US 2004-752792      20040107

PRIORITY APPLN. INFO.:      US 2003-438474P      20030107

ABSTRACT:

The use of bicyclic carbohydrates for the treatment of parasite infections is described. Different bicyclic carbohydrates have been tested in vitro against a number of protozoa. These compds. also have been screened against viruses, tumors, bacteria and fungi. Compound A1, a thiophenyl-containing bicyclic carbohydrate possessed significant activity against *Trypanosoma brucei rhodesiense*, a parasite that causes the lethal sleeping sickness. Compound A2 and Compound A3, bicyclic carbohydrates with halogen containing aryl groups, possessed significant activity against *Leishmania donovani*, a parasite that causes leishmaniasis. Bicyclic carbohydrates in general, and Compound A1, Compound A2 and Compound A3 more specifically, could be possible treatments for the sleeping sickness and leishmaniasis in the future.

SUPPL. TERM:      bicyclic carbohydrate antiprotozoal parasite infection;  
                    *Trypanosoma brucei rhodesiense* inhibition bicyclic  
                    carbohydrate; *Leishmania donovani* inhibition bicyclic  
                    carbohydrate

INDEX TERM:      Human  
                    *Leishmania*  
                    *Leishmania donovani*  
                    Mammalia  
                    Parasite  
                    Protozoa  
                    Protozoacides  
                    *Trypanosoma*  
                    *Trypanosoma rhodesiense*  
                    Trypanosomicides

(bicyclic carbohydrates as antiprotozoal agent for  
treatment of parasite infections)

INDEX TERM:      Carbohydrates, biological studies

ROLE: BSU (Biological study, unclassified); PAC  
(Pharmacological activity); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)  
(bicyclic; bicyclic carbohydrates as antiprotozoal agent  
for treatment of parasite infections)

INDEX TERM:      *Leishmania*  
                    (leishmaniasis from; bicyclic carbohydrates as  
                    antiprotozoal agent for treatment of parasite infections)

INDEX TERM:      Protozoacides  
                    (leishmanicides; bicyclic carbohydrates as antiprotozoal  
                    agent for treatment of parasite infections)

INDEX TERM:      Drug resistance  
                    (protozoal, treatment of; bicyclic carbohydrates as  
                    antiprotozoal agent for treatment of parasite infections)

INDEX TERM:      Infection  
                    (protozoal; bicyclic carbohydrates as antiprotozoal agent  
                    for treatment of parasite infections)

INDEX TERM:      Infection  
                    (trypanosomiasis; bicyclic carbohydrates as antiprotozoal  
                    agent for treatment of parasite infections)

INDEX TERM:      87508-17-6P      727416-80-0P      727416-82-2P

ROLE: BSU (Biological study, unclassified); PAC  
(Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(bicyclic carbohydrates as antiprotozoal agent for treatment of parasite infections)

INDEX TERM: 727416-83-3P

ROLE: BYP (Byproduct); PREP (Preparation)

(bicyclic carbohydrates as antiprotozoal agent for treatment of parasite infections)

INDEX TERM: 100-58-3, Phenyl magnesium bromide 104-88-1,  
p-Chlorobenzaldehyde, reactions 108-98-5, Thiophenol,  
reactions 455-19-6 604-69-3,  $\beta$ -D-Glucose  
pentaacetate 1125-88-8, Benzaldehyde dimethyl acetal  
6921-34-2, Benzylmagnesium chloride 38768-81-9,  
2,3,4,6-Tetra-O-benzyl-D-glucose

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(bicyclic carbohydrates as antiprotozoal agent for treatment of parasite infections)

INDEX TERM: 572-09-8P 2936-70-1P 4196-35-4P 13231-13-5P  
20181-49-1P 23661-28-1P 136034-23-6P 155590-31-1P  
727416-79-7P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)

(bicyclic carbohydrates as antiprotozoal agent for treatment of parasite infections)

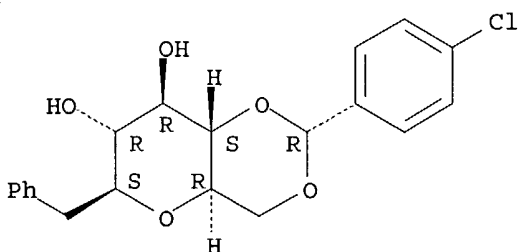
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RN    727416-82-2    REGISTRY  
 ED    Entered STN:    16 Aug 2004  
 CN    D-glycero-D-gulo-Heptitol, 2,6-anhydro-5,7-O-[(R)-(4-chlorophenyl)methylene]-1-deoxy-1-phenyl- (9CI)    (CA INDEX NAME)  
 FS    STEREOSEARCH  
 MF    C20 H21 Cl O5  
 SR    CA  
 LC    STN Files:    CA, CAPLUS, TOXCENTER, USPATFULL  
 DT.CA    Caplus document type:    Patent  
 RL.P    Roles from patents:    BIOL (Biological study); PREP (Preparation); USES (Uses)

## Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2
C4O2-C5O	OCOC3-OC5	6-6	C7O3	591.449.1	1

Absolute stereochemistry.    Rotation (-).



## Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	973	pH 1	(1) ACD
Bioconc. Factor (BCF)	973	pH 4	(1) ACD
Bioconc. Factor (BCF)	973	pH 7	(1) ACD
Bioconc. Factor (BCF)	973	pH 8	(1) ACD
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H donors (HD)	2		(1) ACD
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Solaris V4.76 ((C) 1994-2004 ACD/Labs)

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 INVENTOR(S): Sas, Benedikt; Van Hemel, Johan; Vandekerckhove, Jan; Van Hemel, Johan; Peys, Eric; Van Der Eycken, Johan; Ruttens, Bart; Van Hoof, Steven  
 PATENT ASSIGNEE(S): Kemin Pharma Europe B.V.B.A., USA  
 SOURCE: PCT Int. Appl., 26 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 INT. PATENT CLASSIF.:  
 MAIN: A61K  
 CLASSIFICATION: 1-5 (Pharmacology)  
 Section cross-reference(s): 33  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004062590	A2	20040729	WO 2004-US311	20040107
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KR, KR, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ				

US 2004180838	A1	20040916	US 2004-752792	20040107
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PRIORITY APPLN. INFO.:	US 2003-438474P	20030107
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The use of bicyclic carbohydrates for the treatment of parasite infections is described. Different bicyclic carbohydrates have been tested in vitro against a number of protozoa. These compds. also have been screened against viruses, tumors, bacteria and fungi. Compound A1, a thiophenyl-containing bicyclic carbohydrate possessed significant activity against Trypanosoma brucei rhodesiense, a parasite that causes the lethal sleeping sickness. Compound A2 and Compound A3, bicyclic carbohydrates with halogen containing aryl groups, possessed significant activity against Leishmania donovani, a parasite that causes leishmaniasis. Bicyclic carbohydrates in general, and Compound A1, Compound A2 and Compound A3 more specifically, could be possible treatments for the

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SUPPL. TERM: bicyclic carbohydrate antiprotozoal parasite infection;  
Trypanosoma brucei rhodesiense inhibition bicyclic  
carbohydrate; Leishmania donovani inhibition bicyclic  
carbohydrate

INDEX TERM: Human  
Leishmania  
Leishmania donovani  
Mammalia  
Parasite  
Protozoa  
Protozoacides  
Trypanosoma  
Trypanosoma rhodesiense  
Trypanosomicides  
(bicyclic carbohydrates as antiprotozoal agent for  
treatment of parasite infections)

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ROLE: BSU (Biological study, unclassified); PAC  
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agent for treatment of parasite infections)

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(Preparation); USES (Uses)  
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reactions 455-19-6 604-69-3,  $\beta$ -D-Glucose  
pentaacetate 1125-88-8, Benzaldehyde dimethyl acetal  
6921-34-2, Benzylmagnesium chloride 38768-81-9,  
2,3,4,6-Tetra-O-benzyl-D-glucose  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(bicyclic carbohydrates as antiprotozoal agent for  
treatment of parasite infections)

INDEX TERM: 572-09-8P 2936-70-1P 4196-35-4P 13231-13-5P  
20181-49-1P 23661-28-1P 136034-23-6P 155590-31-1P  
727416-79-7P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)

(bicyclic carbohydrates as antiprotozoal agent for  
treatment of parasite infections)

=>